Headquarters U.S. Air Force

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The BIOPLUME III Natural Attenuation Model

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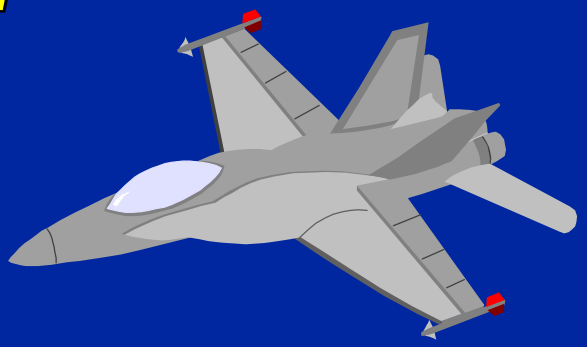
Team Members and Funding

- **Hanadi S. Rifai, Ph.D., P.E.**
  University of Houston
- **Jim Gonzales, Ross Miller**
  AFCEE Tech Transfer Division

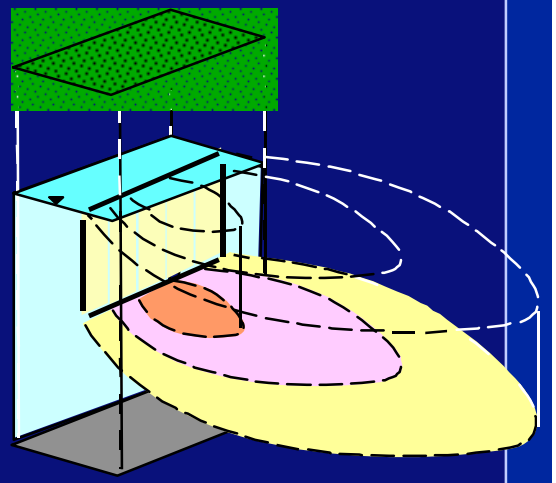
Funded by AFCEE Tech Transfer Division



Natural Attenuation Models

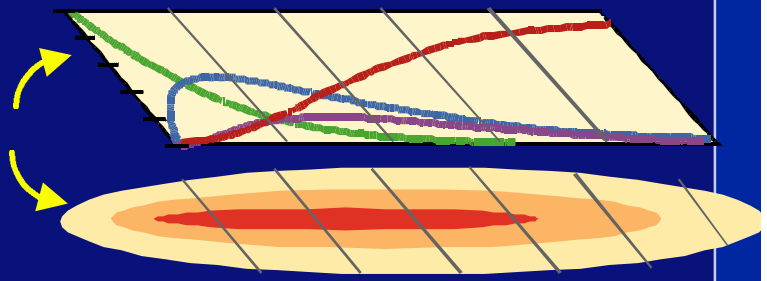
Fuel Sites

- BIOSCREEN *(analytical, two decay options, source decay term)*
- BIOPLUME III *(numerical, electron acceptors)*



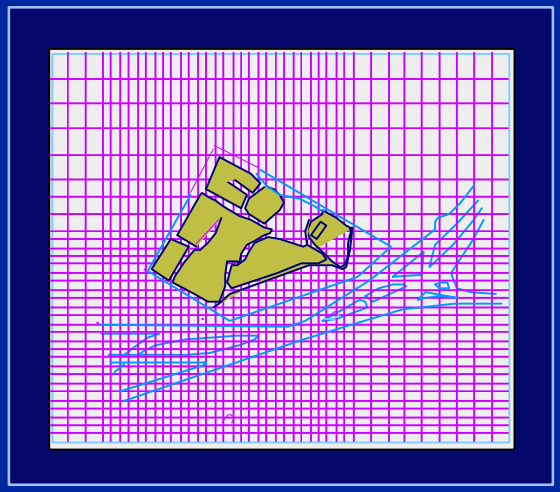
Solvent Sites

- BIOCHLOR *(analytical, sequential reductive dechlorination)*
- RT3D *(complex numerical model)*



Types of Fate and Transport Models

- 1-D vs. 2-D vs. 3-D Advection
- 1-D vs. 2-D vs. 3-D Dispersion
- Deterministic vs. Statistical
- Numerical vs. Analytical
- Transient vs. Steady State
- Constant Source vs. Changing Source



(BIOPLUME III Features)

Model Selection Guidelines

Model Type	Capabilities	Data Needs	Complexity
Hand Calcs:	Advection Only	Simple	
Analytical (BIOSCREEN BIOCHLOR):	Uniform flow Simple source Key NA Processes	Moderate	
Numerical Model (BIOPLUMEIII):	Complex flow Complex sources Pumping	High	

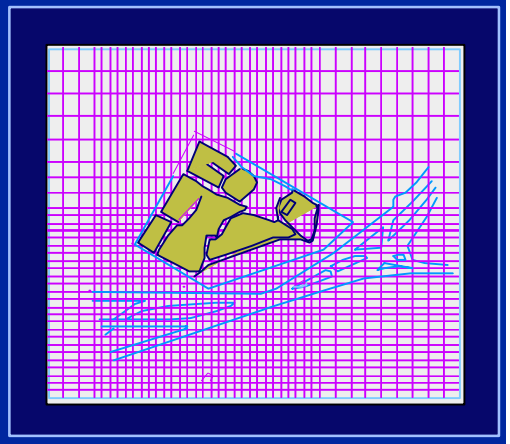
"Gilligan

"Skipper

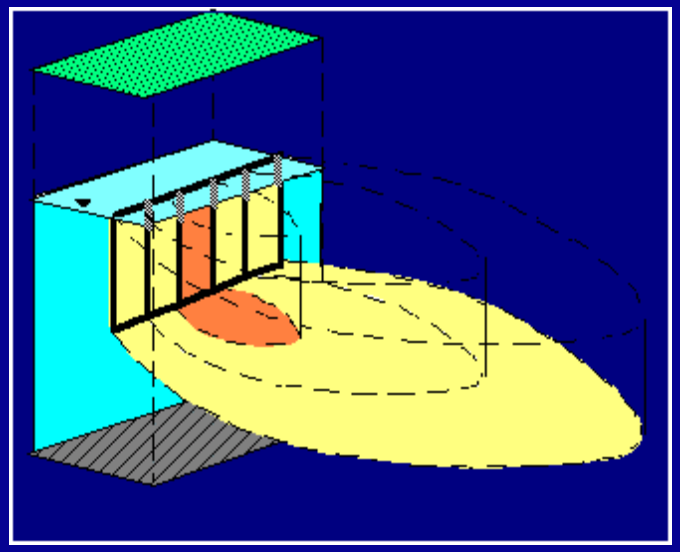
The "Professor

Strengths of Numerical Models such as BIOPLUME III

- Can model **changing flow directions**
- Can simulate complex **changes in source strength** o
- Can handle **pumping wells, streams, springs**, etc.
- Can model **heterogenieties**



Introduction to BIOPLUME III



BIOPLUME III

- Core Model Developed by Hanadi S. Rifai (Univ. of Houston)
- Interface Developed by ZEI/Microengineering
- Funded by AFCEE
- Peer-Reviewed by Blue-Ribbon Panel

BIOPLUME III

- Two-dimensional, finite difference
- Runs on PC in Windows environment
- Enhancement over BIOPLUME II
- Incorporates anaerobic electron acceptors

BIOPLUME III

- Based on the USGS MOC dated July 1989
- Simulates transport of six components
  - contaminant
  - oxygen
  - nitrate
  - iron
  - sulfate
  - carbon dioxide

BIOPLUME III Applicability

- **Primarily used for natural attenuation**
- **Predicts plume extent & receptor concentrations:**

  How far ?

  How long?

BIOPLUME III Limitations

- Does not account for selective or competitive biodegradation
- Simplifies the complex biological redox reactions

BIOPLUME III Conceptual Biodegradation Model

- Sequential Degradation

Oxygen
↘ Nitrate
↘ Iron(III)
↘ Sulfate
↘ Carbon Dioxide

Aerobic and Anaerobic Electron Acceptors

Electron Acceptor	Type of Reaction	Metabolic By-Product	Redox Potential (pH = 7, in volts)	Reaction Preference
Oxygen	Aerobic	CO_2	+ 820	*Most Preferred*
Nitrate	Anaerobic	N_2, CO_2	+ 740	ß
Ferric Iron (solid)	Anaerobic	Ferrous Iron (dissolved)	- 50	ß
Sulfate	Anaerobic	H_2S	- 220	ß
Carbon Dioxide	Anaerobic	Methane	- 240	*Least Preferred*

Redox Reactions

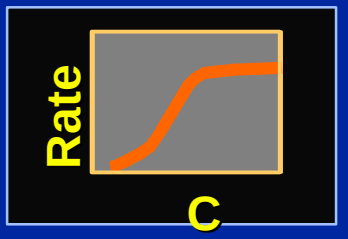
Concept: Combine reduction and oxidation reactions

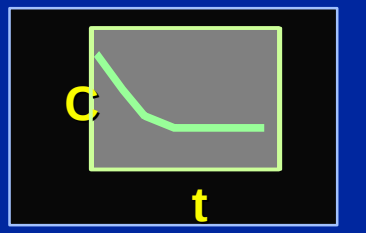
Xylene oxidation reaction:

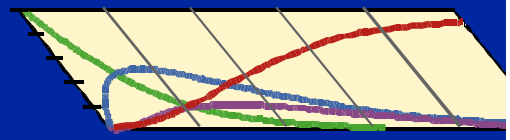
$$C_8H_{10} + 16\ H_2O \rightarrow 8\ CO_2 + 42\ H^+ + 42\ e^-$$

Kinetic Models for in BIOPLUME III

- **Monod/Michaelis-Menton**
  (For any contaminant)(in BIOPLUME III)
- **First Order Decay**
  (For any contaminant) (in BIOSCREEN)
- **Electron Acceptor Limited Biodeg. / ("Instantaneous Reaction)**
  (For BTEX only) (in BIOSCREEN)





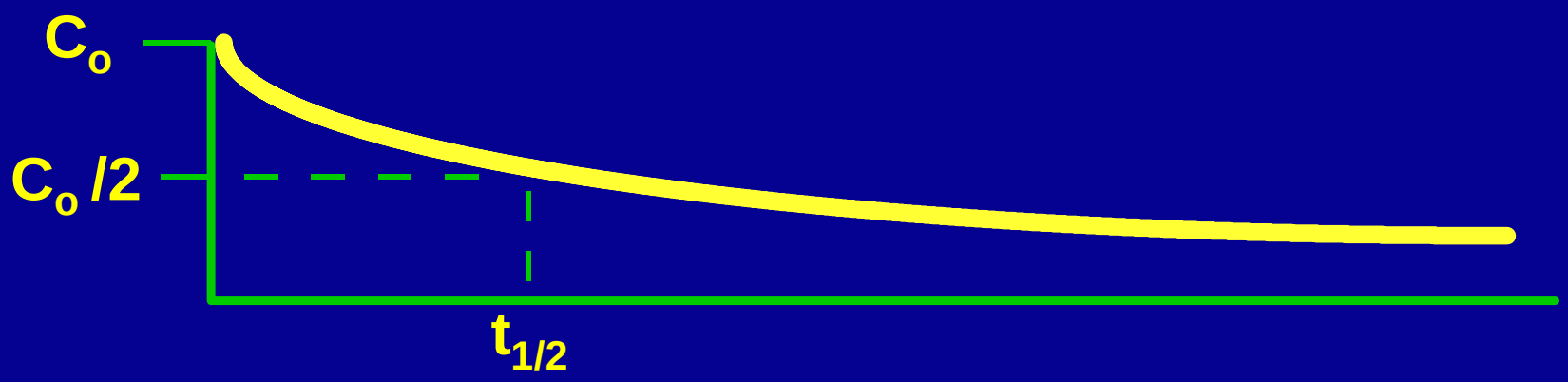


Biodegradation Kinetic Models

First-Order Decay Model

$$C = C_o\, e^{(-kt)}$$

$$t_{1/2} = 0.693 / k$$



Biodegradation Kinetic Models

Instantaneous Reaction Model

$$\Delta C_R = -\frac{O}{F}$$

ΔC_R = Change in contaminant concentration due to biodegradation

O = Concentration of Oxygen

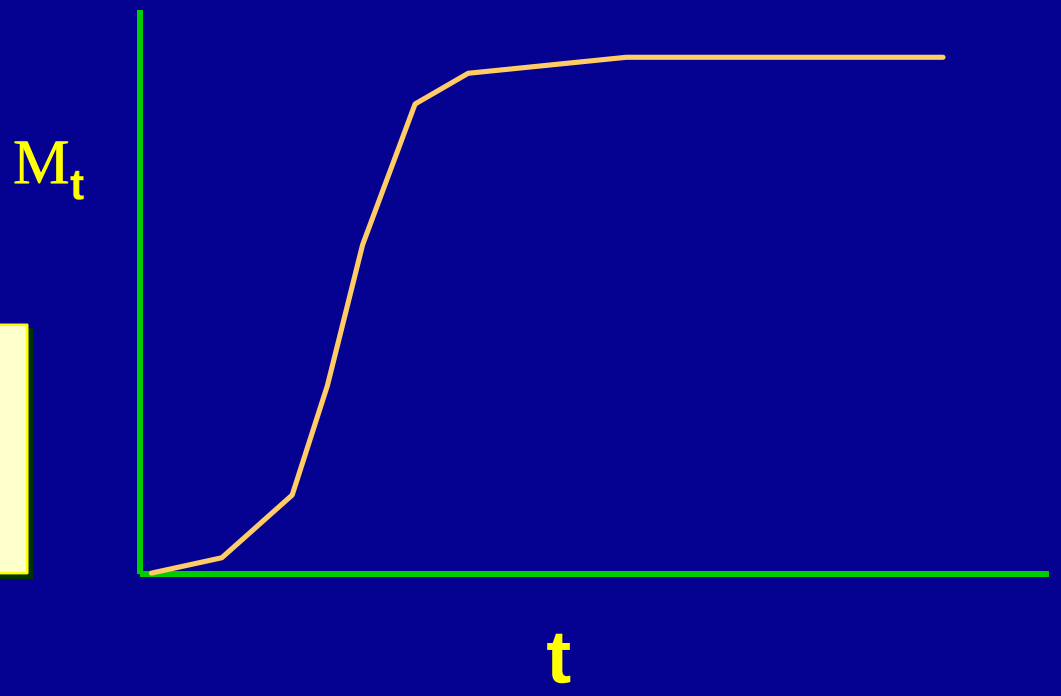
F = Ratio of oxygen to contaminant consumed

Biodegradation Kinetic Models

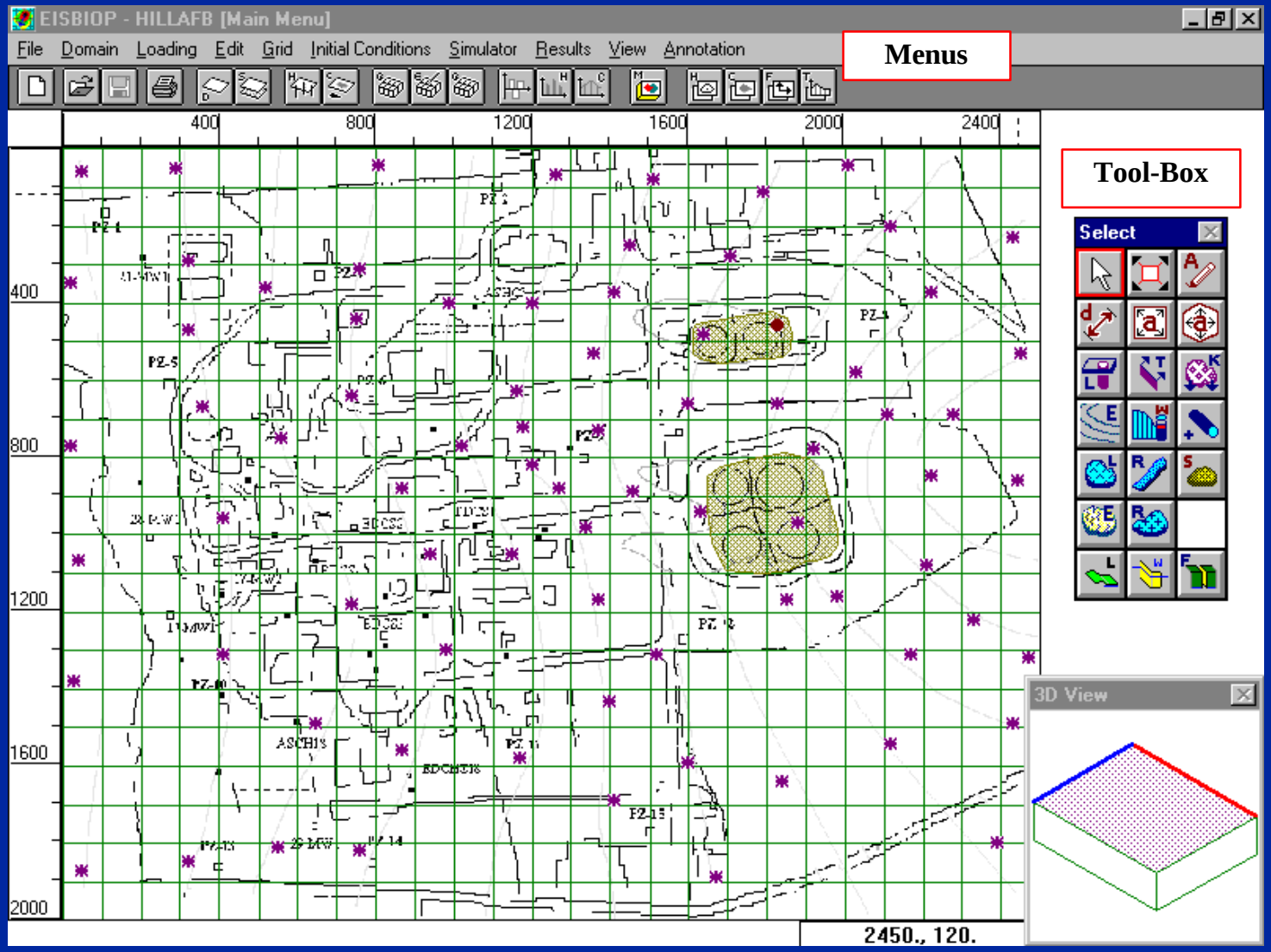
Monod Kinetic Model

$$\mu = \frac{\mu_{max} C}{K_C + C}$$

$$\Delta C = M_t \frac{\mu_{max} C}{K_C + C} \Delta t$$



Graphical User Interface Platform Menu and Toolbox



Modeling Procedures

- Establish model purpose
- Develop conceptual model
- Calibration
- Validation
- Prediction

Where to Get BIOPLUME III

EPA Center for Subsurface Modeling Support (R. S. Kerr Lab)

- **Web:**
  http://www.epa.gov/ada/csmos/models.html
- **Phone**
  (405) 436 8718